

Spin and charge orderings in the atomic limit of the U - V - J model

F Mancini^{1,2}, E Plekhanov^{1,2,3}, and G Sica¹

¹ Dipartimento di Fisica “E.R. Caianiello”, Università degli Studi di Salerno, 84084 Fisciano (SA), Italy

² Unità CNISM di Salerno, Università degli Studi di Salerno, 84084 Fisciano (SA), Italy

³ CNR-SPIN, UoS di Salerno, 84084 Fisciano (SA), Italy

E-mail: plekhanoff@physics.unisa.it

Abstract. In this paper we study a generalization of the 1D Hubbard model by considering density-density and Ising-type spin-spin nearest neighbor (NN) interactions, parameterized by V and J , respectively. We present the $T = 0$ phase diagram for both ferro ($J > 0$) and anti-ferro ($J < 0$) coupling obtained in the narrow-band limit by means of an extension to zero-temperature of the transfer-matrix method. Based on the values of the Hamiltonian parameters, we identify a number of phases that involve orderings of the double occupancy, NN density and spin correlations, being these latter very fragile.

1. Introduction

The Hubbard model (HM) is undoubtedly one of the most studied model in condensed matter physics. In one spatial dimension (1D), the exact Bethe solution for the pure HM is known [1]. During its long history, several extensions to the HM have been proposed. Among them, the inclusion of non-local charge density and/or spin exchange interactions appears to be the most natural choice. Density correlations correspond to an effective finite-range Coulomb interaction (repulsive or attractive) as opposed to the on-site Hubbard U . On the other hand, the spin-spin interaction is believed to be responsible for the interplay between various spin orderings (SDW or ferromagnetism) with strong (triplet) superconducting correlations in a variety of compounds: Sr_2RuO_4 [2], UGe_2 [3], URhGe [4], ZrZn_2 [5] and $(\text{TMTSF})_2\text{X}$ [6] family. Any extension of the HM breaks the integrability, so that either approximate analytic (*e.g.* bosonization) or numerical finite-system methods (*e.g.* Density Matrix Renormalization Group or Quantum Monte Carlo) should be used even in 1D. Bosonization works well in the limit of large bandwidth and predicts several interesting effects like coexistence of spin density wave correlations and (triplet) superconducting ones (for spin exchange interactions [7, 8]) or a transition towards Mott-insulating phases at commensurate fillings (for charge interactions [9]). On the other hand, in the opposite limit of narrow-band width (atomic limit), the extended Hubbard model can be exactly solved by means of any of the two equivalent methods - Transfer Matrix (TM) technique [10] or Composite Operator Method [11, 12]. In the present work we employ a $T \rightarrow 0$ extrapolation of the TM method in order to derive the zero-temperature phase diagram of the extended HM with both nearest-neighbor (NN) charge and spin interactions in the narrow-band limit.

2. Results

The Hamiltonian of the U - V - J system reads as follows:

$$H = \sum_i [-\mu n(i) + UD(i)] + V \sum_i n(i)n(i+1) - J \sum_i S^z(i)S^z(i+1). \quad (1)$$

Here $n(i) \equiv n_\uparrow(i) + n_\downarrow(i)$ denotes the electron density operator at site i , $D(i) \equiv n_\uparrow(i)n_\downarrow(i)$ is the double occupancy at site i while $S^z(i) \equiv (n_\uparrow(i) - n_\downarrow(i))/2$ denotes the z -component of the spin at site i . The Hamiltonian (1) contains only NN term, hence the TM will be a 4×4 matrix. It is easy to check that the TM elements can be calculated through the matrix elements of an auxiliary matrix Z : $T_{ij} = \exp(-\beta Z_{ij})$, where Z is defined as follows:

$$Z = \begin{pmatrix} 0 & -\frac{\mu}{2} & -\frac{\mu}{2} & \frac{U}{2} - \mu \\ -\frac{\mu}{2} & V - \frac{J}{4} - \mu & V + \frac{J}{4} - \mu & \frac{U}{2} + 2V - \frac{3}{2}\mu \\ -\frac{\mu}{2} & V + \frac{J}{4} - \mu & V - \frac{J}{4} - \mu & \frac{U}{2} + 2V - \frac{3}{2}\mu \\ \frac{U}{2} - \mu & \frac{U}{2} + 2V - \frac{3}{2}\mu & \frac{U}{2} + 2V - \frac{3}{2}\mu & U + 4V - 2\mu \end{pmatrix}. \quad (2)$$

In our longer paper [13] we show how to reconstruct the $T = 0$ phase diagram from the TM matrix elements. Here we apply this method to the U - V - J model. We first identify all different matrix elements (we call them energy scales). In the present case these are:

$$\begin{aligned} F^0 &= 0 \\ F^{1/2} &= -\frac{\mu}{2} \\ F_1^1 &= \frac{U}{2} - \mu; \quad F_2^1 = V - \frac{J}{4} - \mu; \quad F_3^1 = V + \frac{J}{4} - \mu \\ F^{3/2} &= \frac{U}{2} + 2V - \frac{3}{2}\mu \\ F^2 &= U + 4V - 2\mu. \end{aligned} \quad (3)$$

In (3) we have already sorted the energy scales based on the values of particle numbers (given by the superscript of F) allowed for a given configuration. In particular, the three energy terms at $n = 1$ can be written as a unique expression as follows:

$$F^1 = A - \mu, \quad (4)$$

where:

$$A \equiv \min\left(\frac{U}{2}, V - \frac{|J|}{4}\right) = \begin{cases} \frac{U}{2}, & \frac{U}{2} < V - \frac{|J|}{4} \\ V - \frac{|J|}{4}, & \frac{U}{2} > V - \frac{|J|}{4} \end{cases}. \quad (5)$$

We choose J as energy scale and explore the phase diagram in the V - U plane. As μ increases, the particle number in the system increases as well. Therefore, for each value of n ($n = 0, \frac{1}{2}, 1, \frac{3}{2}, 2$) we can establish the ranges of the chemical potential, within which μ can change without changing n . Such ranges can be summarized as follows:

$$\begin{aligned} n = 0 : \quad & \mu < \min\left(0, A, x, \frac{2}{3}x\right) & n = 1 : \quad & \max(A, 2A) < \mu < 2x - \max(A, 2A) \\ n = \frac{1}{2} : \quad & 0 < \mu < \min\left(2A, x, \frac{4}{3}x\right) & n = \frac{3}{2} : \quad & \max\left(\frac{2}{3}x, x, 2(x - A)\right) < \mu < 2x \\ n = 2 : \quad & \max\left(x, \frac{4}{3}x, 2x - A, 2x\right) < \mu, \end{aligned} \quad (6)$$

where we introduced $x \equiv \frac{1}{2}(U + 4V)$. Except for the cases $n = 0$ and $n = 2$, which are always possible, the other cases might be incompatible with a given choice of U, V, J . This occurs when the upper-bound of μ becomes lower than the lower-bound. This condition determines the existence of the jump at a given n in the dependence $\mu(n)$. Such conditions are:

$$\begin{aligned} n = \frac{1}{2} \quad & x > 0 \wedge A > 0 \\ n = 1 \quad & 0 < 2A < x \text{ or } A < 0 \wedge A < x \\ n = \frac{3}{2} \quad & x > 0 \wedge A > 0. \end{aligned} \quad (7)$$

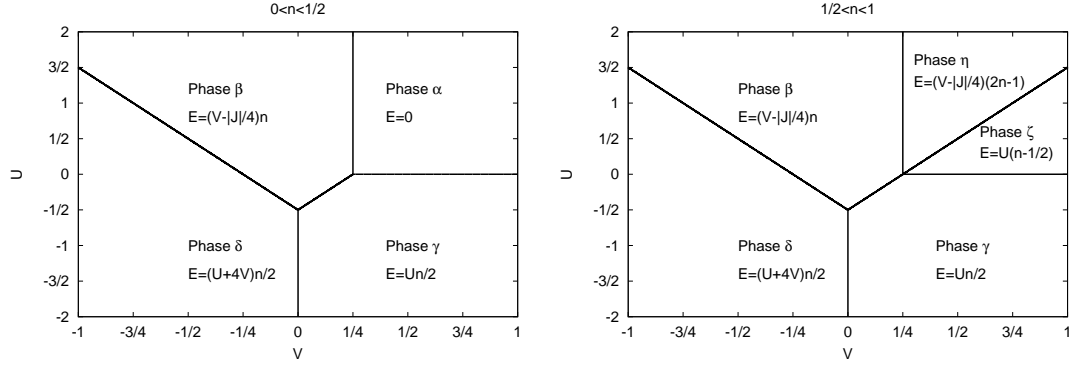


Figure 1. Left panel: Phase diagram in the case $0 < n < \frac{1}{2}$. Right panel: Phase diagram in the case $\frac{1}{2} < n < 1$.

The conditions for the existence of jumps at $n = \frac{1}{2}$ and $n = \frac{3}{2}$ coincide as these values of n are related by the particle-hole relation. Moreover, depending on the values of the Hamiltonian parameters, we can distinguish four cases in the conditions (6):

$$(i) \ x > 0 \wedge A > 0 \quad (ii) \ x > 0 \wedge A < 0 \quad (iii) \ x < 0 \wedge A > x \quad (iv) \ x < 0 \wedge A < x.$$

We can identify three zones in the $V - U$ plane depending on how many jumps there are in the dependence $\mu(n)$:

$$\begin{aligned} (i) \quad & V > \frac{|J|}{4} \wedge U > 0 \\ (ii) \quad & (a) \ \frac{U}{2} > -V - \frac{|J|}{4} \wedge \frac{U}{2} > V - \frac{|J|}{4} \wedge V < \frac{|J|}{4} \quad (b) \ U < 0 \wedge V > 0 \wedge \frac{U}{2} < V - \frac{|J|}{4} \\ (iii) \quad & V < 0 \wedge U < -2V - \frac{|J|}{2}. \end{aligned}$$

The zone i) is characterized by the presence of jumps at all “allowed” values of n : $n = 0, \frac{1}{2}, 1, \frac{3}{2}, 2$, while in the zone ii) the jumps are only at $n = 0, 1, 2$. Finally, in the zone iii), the only jumps present are at $n = 0, 2$. The dependence $\mu(n)$ in the three zones can be summarized as follows:

$$\begin{aligned} i) \quad & \begin{array}{c|c|c|c|c} n=0 & n=\frac{1}{2} & n=1 & n=\frac{3}{2} & n=2 \\ \hline \mu < 0 & 0 < \mu < 2A & 2A < \mu < U+4V-2A & U+4V-2A < \mu < U+4V & U+4V < \mu \end{array} \\ ii) \quad & \begin{array}{c|c|c} n=0 & n=1 & n=2 \\ \hline \mu < A & A < \mu < U+4V-A & U+4V-A < \mu \end{array} \\ iii) \quad & \begin{array}{c|c} n=0 & n=2 \\ \hline \mu < \frac{U}{2}+2V & \frac{U}{2}+2V < \mu \end{array} \end{aligned}$$

We are now in a position to transform from canonical (n fixed) to grand canonical (μ fixed) ensemble. In the zone i) and in the range $0 < n < \frac{1}{2}$, $\mu = 0$ and the free-energy per site (which is a linear function of n) goes from $F_1 = 0$ to $F_2 = -\mu/2|_{\mu=0} = 0$. Therefore, in the above interval F is constantly zero and hence the internal energy per site, which is defined as $E = \frac{1}{N} [\langle H \rangle + \mu \sum_i \langle n(i) \rangle] = F + \mu n$, is zero as well. Analogously, we can determine the behavior of the internal energy as a function of n in the whole range. These findings for the zones i) and ii) are summarized in Tables 1 and 2. In the zone iii), it is easy to verify that $E = (U + 4V)\frac{n}{2}$ for all $0 < n < 2$.

Table 1. Internal energy as a function of particle concentration $E(n)$ for the Zone i).

$0 < n < \frac{1}{2}$	$\frac{1}{2} < n < 1$	$1 < n < \frac{3}{2}$	$\frac{3}{2} < n < 2$
$E = 0$	$E = A(2n - 1)$	$E = (U + 4V)(n - 1) + A(3 - 2n)$	$E = (U + 4V)(n - 1)$

Table 2. Internal energy as a function of particle concentration $E(n)$ for the Zone ii).

$0 < n < 1$	$1 < n < 2$
$E = An$	$E = (U + 4V)(n - 1) + A(2 - n)$

By definition, A takes two different forms depending on whether $\frac{U}{2}$ is greater or not than $V - \frac{|J|}{4}$. This means that everywhere A appears, the two cases should be considered and, therefore, the zones i) and ii) will be further divided in two by the line $\frac{U}{2} = V - \frac{|J|}{4}$. Thanks to the particle-hole symmetry enjoyed by the system, we can consider the phase diagrams just for $n \leq 1$. Two cases can be distinguished: $0 < n < \frac{1}{2}$ and $\frac{1}{2} < n < 1$, together with the particular cases $n = \frac{1}{2}$ and $n = 1$. The two phase diagrams are depicted in Fig. 1. We proceed now to the description of the different phases appearing in the whole phase diagram.

Phase α is located in the range $V > \frac{|J|}{4} \wedge U > 0$ and $0 < n < \frac{1}{2}$. The internal energy is zero because the particles are far apart to activate any of the Hamiltonian terms. The chemical potential vanishes, $\mu = 0$. When $n > \frac{1}{2}$, the former Phase α gives rise to two new phases (η and ζ).

Phase β is located in the range $\frac{U}{2} > |V| - \frac{|J|}{4} \wedge V < \frac{|J|}{4}$. Energy: $E = (V - \frac{|J|}{4})n$ and thus in this phase the singly occupied sites at NN distance interact via density-density and spin-spin interactions. The spin-spin correlation function takes the value:

$$\langle S^z(i)S^z(i+1) \rangle = -\frac{\partial E}{\partial J} = \frac{\text{sign}(J)n}{4}. \quad (8)$$

Hence, if $J < 0$, the system is dominated by antiferromagnetic correlations, while if $J > 0$ the correlations are ferromagnetic. This phase exists in the range $0 < n < 1$. Chemical potential $\mu = V - \frac{|J|}{4}$, NN charge-density correlations $\langle n(i)n(i+1) \rangle = n$. This phase exhibits spontaneous magnetization, uniform in case $J > 0$, or staggered in case $J < 0$.

Phase γ is located in the range $V > 0 \wedge U < 0 \wedge \frac{U}{2} < V - \frac{|J|}{4}$. Energy is $E = \frac{U}{2}n$, and therefore in this phase the doubly occupied sites are separated by at least one empty site. This phase exists in the range $0 < n < 1$. Chemical potential $\mu = \frac{U}{2}$. The only non-zero correlation function is $\langle D(i) \rangle = n/2$.

Phase δ is located in the range $V < 0 \wedge \frac{U}{2} < -V - \frac{|J|}{4}$ for all $0 < n < 2$. The energy: $E = (U + 4V)\frac{n}{2}$ and thus, in this phase, the doubly occupied sites are placed at the NN distance. Chemical potential $\mu = \frac{U}{2} + 2V$. The only non-zero correlation functions are $\langle D(i) \rangle = n/2$, $\langle n(i)n(i+1) \rangle = 2n$ and $\langle D(i)D(i+1) \rangle = n/2$.

Phase η is located in the range $V > \frac{|J|}{4} \wedge \frac{U}{2} > V - \frac{|J|}{4}$ and $\frac{1}{2} < n < 1$. The energy $E = (V - \frac{|J|}{4})(2n - 1)$. This is the second phase with magnetic correlations and is similar to the adjacent Phase β in the sense that in both phases density-density and spin-spin correlations are present, although the expressions for the correlation functions are different: $\langle n(i)n(i+1) \rangle = 2n - 1$, $\langle S^z(i)S^z(i+1) \rangle = \frac{\text{sign}(J)}{4}(2n - 1)$. Chemical potential $\mu = 2(V - \frac{|J|}{4})$. There also exists spontaneous magnetization, uniform in case $J > 0$, or staggered in case $J < 0$.

Phase ζ is located in the range $\frac{U}{2} > V - \frac{|J|}{4} \wedge U > 0$ and $\frac{1}{2} < n < 1$. The energy $E = U(n - \frac{1}{2})$. This phase is similar to the Phase γ in the sense explained above. Chemical potential $\mu = U$, while the only non-vanishing correlation function is $\langle D(i) \rangle = n - 1/2$.

The phase boundaries for the phases at $n > 1$ are identical to those at $n < 1$ and the expressions for the internal energy can be obtained from those at $n < 1$ by invoking the particle-hole symmetry:

$$E(2 - n) = E(n) + (U + 4V)(1 - n), \quad (9)$$

while for the chemical potential the particle-hole relation states:

$$\mu(2 - n) = (U + 4V) - \mu(n). \quad (10)$$

3. Conclusions

In this work we present an original method for extrapolating the TM technique at $T = 0$ and use it to obtain the exact $T = 0$ phase diagram of the extended Hubbard U - V - J model in the narrow-band limit. Depending on the values of the Hamiltonian parameters, the orderings involve double occupancy, NN density and spin correlations. We note that the phase diagram boundaries do not depend on the sign of J , although the spin correlations do. The spin correlations appear to be rather fragile in our model: the Ising term in the Hamiltonian acts only if the NN sites are singly occupied. However, in the same conditions the V term is also active, while the U term tends to create either doubly occupied or empty sites (depending on the sign of U). That is why, when either V is large and positive or U is large and negative the spin correlations are completely suppressed. The introduction of J affects only the phases (β and η) where the sites are singly occupied. In these phases, for $J = 0$ [14, 12], the spins are not ordered while, if $J \neq 0$, a ferromagnetic or antiferromagnetic order is established depending on the sign of J .

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